

UPRF-94-408

# A Complete Perturbative Expansion for Constrained Quantum Dynamics

P. Maraner

*Dipartimento di Fisica, Università di Parma,  
and INFN, Gruppo collegato di Parma,  
Viale delle Scienze, 43100 Parma, Italy*

August 1994

## Abstract

A complete perturbative expansion for the Hamiltonian describing the motion of a quantomechanical system constrained to move on an arbitrary submanifold of its configuration space  $R^n$  is obtained.

# 1 Introduction

The quantomechanical description of constrained systems is extremely important in physics and since the early days of quantum mechanics several techniques have been developed to deal with this matter. A fundamental contribution has been given by Dirac [1]. His idea, geometrical in nature, consists in removing the redundant degrees of freedom by the construction of a consistent hamiltonian formalism for the constrained classical theory and proceeding then to its quantization. Other noteworthy approach have been developed by Schwinger, Peierls by using variational arguments and by De Witt, Faddeev, Popov by means of lagrangian formalism and of path integral techniques. The common feature to all this methods, to which we will refer as *formal methods*, is that *the reduction of the dynamics to the constraint surface is performed before the quantization of the system*. Although in many cases this is the only way to proceed, it often introduces non physical ambiguities causing some pure quantomechanical effects to be ignored.

Let us consider for example a particle constrained to move on an arbitrary surface  $\Sigma$  embedded in the three-dimensional euclidean space  $R^3$ . The reduction of the classical theory is straightforward. Introducing  $x^1, x^2$  coordinates parametrizing the surface and denoting by  $g_{\mu\nu}$ ,  $\mu, \nu = 1, 2$ , the metric induced on  $\Sigma$  from  $R^3$ , the system is described by the lagrangian  $\mathcal{L} = \frac{1}{2}g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu$ . Defining the generalized momenta  $p_\mu = \partial\mathcal{L}/\partial\dot{x}^\mu$  we obtain the Hamiltonian  $\mathcal{H} = \frac{1}{2}g^{\mu\nu}p_\mu p_\nu$ ,  $g^{\mu\nu}$  denoting the inverse of the metric. The quantization of  $\mathcal{H}$  contains ordering ambiguities which are not completely removed by the required covariance of the theory. As first observed by De Witt [2], in constructing the Hamiltonian operator we are free to add to minus one half the laplacian  $\Delta$  a term proportional to the scalar curvature  $R$  of the surface,

$$\mathcal{H} = -\frac{1}{2}\Delta + \alpha R. \quad (1)$$

Different quantization schemes produces different values for the constant  $\alpha$ .  $\alpha$  may not be unambiguously determined, depending essentially on an ordering choice. On the other hand the reduction of the motion of a particle to a surface is by no means an academic problem. Devices producing the confinement of electrons on a plane are widely studied in physics, for example in the Quantum Hall Effect's context [3], and we may think to use the

same techniques to constraint a particle on an arbitrary surface  $\Sigma$ . How to determine then the constant  $\alpha$ ? In addressing the solution of the problem it is convenient to give up the formal treatment of the constraint, thinking instead at the physical mechanism producing the confinement of the particle to the surface. The analysis of devices used in the Quantum Hall Effect stuff, suggests the confinement to be produced by a potential presenting a deep minimum in correspondence of the constraint surface and depending only on the coordinate normal to it [3, 4, 5]. Moving along this line H. Jensen and H. Koppe [6] have first given a realistic description of the motion of a particle on a surface embedded in  $R^3$ . In accordance with Heisenberg's principle the confinement causes the particle to fluctuate very strongly in the direction normal to the surface so that the spectrum of the system is described in first approximation by that of the confining potential. In correspondence of each level the effective Hamiltonian describing the motion along the surface may then be unambiguously obtained as (see Ref.[6] and the discussion below)

$$\mathcal{H} = -\frac{1}{2}\Delta + \frac{1}{4}R - \frac{1}{8}\xi^2, \quad (2)$$

where  $\xi$  is the extrinsic mean curvature of the surface  $\Sigma$ . The analysis have to be completed by considering the interactions between the degrees of freedom normal to the surface and those parallel to it. The case of a wire embedded in  $R^3$  has also been considered by many authors [7].

From this simple example we learn that the operation of reducing the dynamics and quantizing a constrained system do not in general commute and that performing the former before the latter may produce the appearance of unphysical ambiguities and the neglecting of contributions connected to the extrinsic geometrical properties of the constraint surface.

In this paper we present a complete perturbative description of a system constrained to move on a submanifold of its configuration space  $R^n$  by a confining potential  $V_C$ . Generalizing the example of the surface embedded in  $R^3$  we require  $V_C$  to satisfy two very general conditions

- C1)  $V_C$  presents a deep minimum in correspondence of the constraint surface,
- C2)  $V_C$  depends only on coordinates normal to the constraint surface.

In our scheme *the reduction of the dynamics to the constraint surface is performed after the quantization of the system*. Adapting coordinates to the

constraint in section 2, a complete perturbative expansion for the Hamiltonian describing the motion of the system is obtained in section 3. In accordance with Heisenberg principle the zero order term of the expansion takes into account the fluctuations of the system in the directions normal to the constraint surface. The first order term, already discussed in Refs.[4, 5, 8], describes the effective constrained dynamics while the rest of the perturbative expansion describes the interactions between normal and effective degrees of freedom. We want to point out that the constrained quantum dynamics is characterized by the whole expansion, the effective dynamics on the constraint surface representing only the leading term. Contrary to what happens in the classical description, the explicit form of the potential realizing the constraint leaves traces in the effective dynamics and in the spectrum of the system and therefore may not be neglected. This is illustrated by two example in sections 5 and 6. Section 7 contains our conclusions.

## 2 Geometrical Preliminary

In the sequel we identify the constraint surface with a smooth  $m$ -dimensional submanifold  $M$  of the configuration space  $R^n$ . Denoting by  $\Phi : M \rightarrow R^n$  the embedding of  $M$  in  $R^n$  and by  $\mathbf{n}^1(x), \mathbf{n}^2(x), \dots, \mathbf{n}^{n-m}(x)$ , a smooth assignment of  $(n-m)$  orthonormal vectors normal to  $M$  in every point  $x \in M$ , an *adapted coordinates frame* may be introduced by using coordinates  $x^\mu, \mu = 1, \dots, m$ , on  $M$ , plus the distances  $y^i, i = 1, \dots, n-m$ , along the geodetics leaving  $M$  with speed  $\mathbf{n}^i$ . In a “sufficiently close” neighbourhood of  $M$  the frame  $\{x^\mu, y^i; \mu = 1, \dots, m, i = 1, \dots, n-m\}$  is well defined and its relation with the Cartesian coordinates  $\mathbf{r} = (r^1, \dots, r^n)$  of  $R^n$  is given by

$$\mathbf{r} = \Phi(x^\mu) + y^i \mathbf{n}^i(x^\mu). \quad (3)$$

It is important to realize that the embedding of  $M$  in  $R^n$  is completely characterized by the assignment of some tensorial quantities on  $M$  [9]. In an adapted coordinates frame these may be easily constructed as follows

$$\begin{aligned} g_{\mu\nu} &= \mathbf{t}_\mu \cdot \mathbf{t}_\nu && \text{induced metric (first fundamental form)} \\ \alpha_{\mu\nu}^i &= \mathbf{n}^i \cdot \partial_\nu \mathbf{t}_\mu && \text{second fundamental form} \\ A_\mu^{ij} &= \mathbf{n}^i \cdot \partial_\mu \mathbf{n}^j && \text{normal fundamental form} \end{aligned}$$

where  $\mathbf{t}_\mu = \partial_\mu \Phi$  denote the tangent vectors to  $M$  associated with the chosen coordinate frame and the dot the standard scalar product in  $R^n$ .

The choice of an adapted coordinates frame is obviously not unique. An arbitrary coordinates transformation on  $M$  as well as a point dependent rotation of the normal vectors  $\mathbf{n}^i(x)$  transforms an adapted coordinates frame into an adapted coordinates frame. Whereas varying the choice of the coordinates  $x^\mu$  causes  $g_{\mu\nu}$ ,  $\alpha_{\mu\nu}^i$  and  $A_\mu^{ij}$  to transform as tensors of  $M$ , the variation of normal vectors  $\mathbf{n}^i(x)$  by a rotation  $R^{kl}(x)$  makes  $\alpha_{\mu\nu}^i$  to transform as a  $SO(n-m)$  vector but  $A_\mu^{ij}$  as a  $SO(n-m)$  gauge connection

$$A_\mu^{ij} \longrightarrow \mathcal{R}^{ik} A_\mu^{kl} \mathcal{R}^{jl} + \mathcal{R}^{ik} \partial_\mu \mathcal{R}^{jk}. \quad (4)$$

The normal fundamental form  $A_\mu^{ij}$  actually represents the connection induced by  $R^n$  on the normal bundle of  $M$ ,  $TM^\perp$ .

The metric  $G_{IJ}$ ,  $I, J = 1, \dots, n$  of  $R^n$  in the adapted coordinates frame  $\{x^\mu, y^i\}$  writes

$$G_{IJ} = \begin{pmatrix} \gamma_{\mu\nu} + y^k y^l A_\mu^{kh} A_\nu^{lh} & y^k A_\mu^{jk} \\ y^k A_\nu^{ik} & \delta^{ij} \end{pmatrix} \quad (5)$$

where, introducing the matrix  $\eta$  by  $\eta_\nu^\mu = y^i g^{\mu\rho} \alpha_{\rho\nu}^i$ , the matrix  $\gamma$  may be written as

$$\gamma_{\mu\nu} = g_{\mu\rho} (\mathbf{1} - \eta)_\sigma^\rho (\mathbf{1} - \eta)_\nu^\sigma \quad (6)$$

The determinant  $|G|$  of  $G_{IJ}$  coincides with that of the matrix  $\gamma$ ,  $|\gamma|$ , and the inverse of the metric tensor may be calculated as

$$G^{IJ} = \begin{pmatrix} \gamma^{\mu\nu} & \gamma^{\mu\rho} y^k A_\rho^{kj} \\ \gamma^{\nu\rho} y^k A_\rho^{ki} & \delta^{ij} + y^k y^l A_\rho^{ik} A_\sigma^{jl} \gamma^{\rho\sigma} \end{pmatrix}. \quad (7)$$

### 3 The Perturbative Expansion

We come now to the dynamical aspect of the problem. The quantization of the system is performed very easily and unambiguously in  $R^n$ , before considering the constraint. In a cartesian coordinates frame  $\{r^I; I = 1, \dots, n\}$ , dynamics is described by

$$\mathcal{H} = -\frac{1}{2} \partial_I \partial_I + V_C, \quad (8)$$

where  $V_C$  is the potential realizing the constraint.  $\mathcal{H}$  acts on wavefunctions  $\psi \in \mathcal{L}^2(R^n)$  normalized with the condition

$$\int |\psi|^2 dr^n = 1. \quad (9)$$

In an *adapted coordinates frame*  $\{x^\mu, y^i; \mu = 1, \dots, m, i = m+1, \dots, n\}$  Hamiltonian (8) takes the form

$$\mathcal{H} = -\frac{1}{2|G|^{1/2}} \partial_I G^{IJ} |G|^{1/2} \partial_J + V_C, \quad (10)$$

and the normalization condition (9) transforms to

$$\int |\psi|^2 |G|^{1/2} dx^m dy^{(n-m)} = 1. \quad (11)$$

Since we are looking for an effective dynamics on the submanifold  $M$  we find it natural to perform a similitude transformation in such a way that wave functions are correctly normalized in  $\mathcal{L}^2(M)$  instead of  $\mathcal{L}^2(R^n)$ . The aim is achieved by

$$\begin{aligned} \psi &\rightarrow \frac{|g|^{1/4}}{|G|^{1/4}} \psi \\ \mathcal{H} &\rightarrow \frac{|g|^{1/4}}{|G|^{1/4}} \mathcal{H} \frac{|G|^{1/4}}{|g|^{1/4}} \end{aligned} \quad (12)$$

where  $|g|$  denotes the determinant of the metric  $g_{\mu\nu}$  induced on  $M$ . Considering the explicit form (7) of the inverse metric  $G^{IJ}$  and introducing  $\hat{\partial}_\mu = \partial_\mu + iA_\mu^{ij} L_{ij}/2$ , where  $L_{ij} = -i(y^i \partial_j - y^j \partial_i)$  are the  $SO(n-m)$  generators, Hamiltonian (10) takes the quite complicated form

$$\mathcal{H} = -\frac{1}{2|\gamma|^{1/4}} \partial_i |\gamma|^{1/2} \partial_i \frac{1}{|\gamma|^{1/4}} - \frac{1}{2|g|^{1/4} |\gamma|^{1/4}} \hat{\partial}_\mu \gamma^{\mu\nu} |\gamma|^{1/2} \hat{\partial}_\nu \frac{|g|^{1/4}}{|\gamma|^{1/4}} + V_C. \quad (13)$$

At this point, and only at this point, the constraint is imposed by considering conditions  $C1$  and  $C2$ . Condition  $C1$  assures that the potential  $V_C$  may be replaced by its power expansion around the minimum  $\vec{y} = 0$ . Condition  $C2$  states that there exist an adapted coordinates frame in which  $V_C$  only depends on the normal coordinates  $\vec{y}$ . Without loss of generality the

constant term of the expansion may be neglected and the quadratic term diagonalized by means of a point independent rotation in the normal space

$$V_C(\vec{y}) = \frac{1}{2\epsilon^2}\omega^{i^2}y^{i^2} + a_{ijk}y^iy^jy^k + b_{ijkl}y^iy^jy^ky^l + \dots \quad (14)$$

The scale of the proper frequencies  $\omega^i$  has been readsorbed in the adimensional parameter  $\epsilon^{-1}$ . The smaller  $\epsilon$  the deeper is the minimum of  $V_C$  and the more the system is squeezed on the constraint surface.

$\epsilon$  appears as a natural perturbative parameter in the theory and, rescaled the normal coordinates by  $\vec{y} \rightarrow \epsilon^{1/2}\vec{y}$ , a perturbative theory may be set up by expanding Hamiltonian (13) in powers of  $\epsilon$

$$\begin{aligned} \epsilon\mathcal{H} = & H^{(0)} + \epsilon H^{(1)} + \epsilon^{3/2}H^{(3/2)} + \epsilon^2H^{(2)} + \dots + \\ & + \epsilon^{5/2}a_{ijk}y^iy^jy^k + \epsilon^3b_{ijkl}y^iy^jy^ky^l + \dots \end{aligned} \quad (15)$$

The constants  $a_{ijk}$ ,  $b_{ijkl}$ , ... appearing in the expansion of the confining potential are such that the second, the third and further terms of the right hand side of (14) are small compared to the first term and in this sense are  $\epsilon$ -dependent. In practical application they appear in the perturbative expansion as independent parameter so that, for example,  $\epsilon^{5/2}a_{ijk}y^iy^jy^k$  is not in general of order  $\epsilon^{5/2}$ , its magnitude depending on the explicit form of the potential  $V_C$ . The zero and first order terms of expansion (15) has been extensively discussed in Ref.[4].

In accordance with Heisenberg principle the zero order dynamics depends only on normal degrees of freedom,

$$H^{(0)} = \frac{1}{2} \left( -\partial_i\partial_i + \omega^{i^2}y^{i^2} \right), \quad (16)$$

describing a system of  $(n - m)$  uncoupled harmonic oscillators with frequencies  $\omega^{m+1}, \dots, \omega^n$ .

More surprising results follow from the analysis of the first order term,

$$H^{(1)} = -\frac{1}{2g^{1/2}} \left( \partial_\mu + \frac{i}{2}A_\mu^{ij}L_{ij} \right) g^{\mu\nu}g^{1/2} \left( \partial_\nu + \frac{i}{2}A_\nu^{kl}L_{kl} \right) + Q^{(1)}(x), \quad (17)$$

where the potential  $Q^{(1)}$  may be expressed in terms of the intrinsic scalar curvature  $R$  and the extrinsic mean curvature  $\xi$  as

$$Q^{(1)}(x) = \frac{1}{4}R(x) - \frac{m^2}{8}\xi^2(x). \quad (18)$$

Aside from the potential term  $Q^{(1)}$ ,  $H^{(1)}$  is proportional to the Laplace operator on  $M$  coupled to the motion in normal directions by means of the minimal interaction with the gauge field  $A_\mu^{ij}L_{ij}/2$ . It is therefore resonable to expect that in a perturbative picture  $H^{(1)}$  describes the effective dynamics on  $M$ . This has actually been found in Ref.[4]. The surprising result, unexpected and unrecoverable by means of a formal treatment of constraints, is that the effective dynamics is coupled with gauge fields and quantum potentials induced by the intrinsic and extrinsic geometrical properties of the constraint surface. The physical relevance of such a geometry-induced dynamical structure has been recently discussed in Ref.[5], showing how this phenomenon is observable in the effective rotational motion of some simple polyatomic molecules.

Since we are interested in a realistic description of a constrained microscopic system we never consider the limit  $\epsilon \rightarrow 0$ .  $\epsilon$  is a small but finite parameter, its magnitude depending on the characteristics of the system under consideration. It is therefore very important to know the explicit expression of further terms of expansion (15) in order to predict the spectrum of the system with an adequate precision.

To evaluate the explicit expression of the generic term of the expansion (15) we start by observing that the first and second terms of Hamiltonian (13) may be rewritten solely in terms of  $\gamma^{\mu\nu}$  and  $\ln |\mathbf{1} - \eta|$  as

$$-\frac{1}{2|\gamma|^{1/4}}\partial_i|\gamma|^{1/2}\partial_i\frac{1}{|\gamma|^{1/4}} = -\frac{1}{2}\partial_i\partial_i + \frac{1}{4}(\partial_i\partial_i \ln |\mathbf{1} - \eta|) + \frac{1}{8}(\partial_i \ln |\mathbf{1} - \eta|)(\partial_i \ln |\mathbf{1} - \eta|),$$

and

$$-\frac{1}{2|g|^{1/4}|\gamma|^{1/4}}\hat{\partial}_\mu\gamma^{\mu\nu}|\gamma|^{1/2}\hat{\partial}_\nu\frac{|g|^{1/4}}{|\gamma|^{1/4}} = -\frac{1}{2}\hat{\nabla}_\mu\gamma^{\mu\nu}\hat{\nabla}_\nu + \frac{1}{4}\left(\hat{\nabla}_\mu\gamma^{\mu\nu}\hat{\nabla}_\nu \ln |\mathbf{1} - \eta|\right) + \frac{1}{8}\gamma^{\mu\nu}\left(\hat{\nabla}_\mu \ln |\mathbf{1} - \eta|\right)\left(\hat{\nabla}_\nu \ln |\mathbf{1} - \eta|\right),$$

where, denoting by  $\nabla_\mu$  the covariant derivative associated with the connection induced on  $M$ ,

$$\hat{\nabla}_\mu = \nabla_\mu + \frac{i}{2}A_\mu^{ij}L_{ij}. \quad (19)$$



It is very convenient to introduce the matrices

$$\eta_{(N)}^{\mu\nu} = (N+1)g^{\mu\rho_1}y^{i_1}\alpha_{\rho_1\sigma_1}^{i_1}g^{\sigma_1\rho_2}\dots y^{i_N}\alpha_{\rho_N\sigma_N}^{i_N}g^{\sigma_N\nu}, \quad (20)$$

$\eta_{(0)}^{\mu\nu} = g^{\mu\nu}$ . The expansion in  $\epsilon$  of  $\gamma^{\mu\nu}$  and  $\ln|\mathbf{1} - \eta|$  may then be computed as

$$\gamma^{\mu\nu} = \sum_{N=0}^{\infty} \epsilon^{N/2} \eta_{(N)}^{\mu\nu}, \quad (21)$$

$$\ln|\mathbf{1} - \eta| = - \sum_{N=1}^{\infty} \frac{\epsilon^{N/2}}{N} \text{tr} [\eta^N]. \quad (22)$$

The evaluation of the  $N/2$ -order term of the perturbative expansion (15) reduces so to a matter of simple algebra yielding

$$H^{(N/2)} = -\frac{1}{2}\hat{\nabla}_\mu \eta_{(N-2)}^{\mu\nu} \hat{\nabla}_\nu + Q^{(N/2)}, \quad (23)$$

$N \geq 2$ , where the potentials  $Q^{(N/2)}$  may be written as

$$\begin{aligned} Q^{(1)} &= \frac{1}{8} \text{tr} [\partial_i \eta] \text{tr} [\partial_i \eta] - \frac{1}{4} \text{tr} [\partial_i \eta \partial_i \eta], \\ Q^{(3/2)} &= \frac{1}{4} \text{tr} [\partial_i \eta] \text{tr} [\eta \partial_i \eta] - \frac{1}{2} \text{tr} [\eta \partial_i \eta \partial_i \eta] - \frac{1}{4} \text{tr} [\hat{\nabla}_\mu g^{\mu\nu} \hat{\nabla}_\nu \eta], \end{aligned}$$

and for  $N \geq 4$

$$\begin{aligned} Q^{(N/2)} &= \sum_{K=0}^{N-2} \left\{ \frac{1}{8} \text{tr} [\eta^K \partial_i \eta] \text{tr} [\eta^{N-K-2} \partial_i \eta] - \frac{1}{4} \text{tr} [\eta^{N-2} \partial_i \eta \partial_i \eta] \right\} + \\ &- \sum_{K=0}^{N-3} \frac{1}{4} \text{tr} [\eta^{N-K-3} \hat{\nabla}_\mu \eta_{(K)}^{\mu\nu} \hat{\nabla}_\nu \eta + (N-K-3) \eta_{(K)}^{\mu\nu} \eta^{N-K-4} (\hat{\nabla}_\mu \eta) (\hat{\nabla}_\nu \eta)] + \\ &+ \sum_{K=0}^{N-4} \sum_{L=1}^{N-K-3} \frac{1}{8} \eta_{(K)}^{\mu\nu} \text{tr} [\eta^{L-1} (\hat{\nabla}_\mu \eta)] \text{tr} [\eta^{N-K-L-3} (\hat{\nabla}_\nu \eta)]. \end{aligned}$$

It is remarkable that the perturbative expansion of the Hamiltonian of the system is completely written in terms of the induced metric  $g_{\mu\nu}$ , the second fundamental form  $\alpha_{\mu\nu}^i$ , its first and second covariant derivative  $\nabla_\rho \alpha_{\mu\nu}^i$ ,  $\nabla_\sigma \nabla_\rho \alpha_{\mu\nu}^i$  and the normal fundamental form  $A_\mu^{ij}$ .  $A_\mu^{ij}$  appears in the perturbative expansion only by means of the minimal coupling (19).

## 4 Spectrum and Effective Dynamics

To evaluate the spectrum of the system we proceed now by means of the standard Raleigh-Schrödinger perturbation theory. We identify  $H^{(0)}$  with the unperturbed Hamiltonian and the rest of expansion (15) with the perturbation  $\mathcal{P}_\epsilon$ ,

$$\epsilon\mathcal{H} = H^{(0)} + \mathcal{P}_\epsilon. \quad (24)$$

As stated in the previous section,  $H^{(0)}$  represents a system of  $(n - m)$  uncoupled harmonic oscillator. We denote by  $\chi_{\mathcal{N}}(\vec{y})$  its eigenfunctions, having collected the harmonic oscillator quantum numbers  $n_{m+1}, \dots, n_n$  in the multiindex  $\mathcal{N} = (n_{m+1}, \dots, n_n)$ . The corresponding eigenvalues are given by  $E^{(0)} = \sum_i \omega^i (n_i + 1/2)$ . The spectrum is degenerate every time the frequencies  $\omega^i$  satisfy linear conditions in the integer field. The zero order eigenfunctions corresponding to an energy  $E^{(0)}$  are given by

$$\psi_{\mathcal{N}}^{(0)}(\vec{x}, \vec{y}) = \phi_{\mathcal{N}}(\vec{x}) \chi_{\mathcal{N}}(\vec{y}) \quad (25)$$

and present an infinite degeneracy given by the presence of the arbitrary function of  $\vec{x}$ ,  $\phi_{\mathcal{N}}(\vec{x})$ , beside that labelled by the multiindex corresponding to the energy  $E^{(0)}$ .

The first order correction to  $E^{(0)}$ ,  $E^{(1)}$ , is obtained by diagonalizing the perturbation on degenerate states, that is by solving the Schrödinger equation

$$\mathcal{H}^{E^{(0)}} \phi(\vec{x}) = E^{(1)} \phi(\vec{x}), \quad (26)$$

where the Hamiltonian  $\mathcal{H}^{E^{(0)}}$  is obtained by bracketing the order  $\epsilon$  term of  $\mathcal{P}_\epsilon$ ,  $H^{(1)}$ , between the harmonic oscillator states corresponding to  $E^{(0)}$  and  $\phi(\vec{x})$  is a vector wavefunction having as component the  $\phi_{\mathcal{N}}(\vec{x})$  with energy  $E^{(0)}$ . The explicit expression of  $\mathcal{H}^{E^{(0)}}$  is

$$\mathcal{H}^{E^{(0)}} = -\frac{1}{2g^{1/2}}(\mathbf{1}\partial_\mu + iA_\mu)g^{\mu\nu}g^{1/2}(\mathbf{1}\partial_\nu + iA_\nu) + Q^{(1)}(\vec{x}) + \bar{Q}^{(1)}(\vec{x}) \quad (27)$$

with

$$A_\mu = \frac{1}{2}A_\mu^{ij}\langle L_{ij} \rangle, \quad (28)$$

$$\bar{Q}^{(1)} = \frac{1}{8}g^{\mu\nu}A_\mu^{ij}A_\nu^{kl}(\langle L_{ij}L_{kl} \rangle - \langle L_{ij} \rangle \langle L_{kl} \rangle), \quad (29)$$

where  $\langle L_{ij} \rangle$  and  $\langle L_{ij} L_{kl} \rangle$  denote the matrices obtained by bracketing  $L_{ij}$  and  $L_{ij} L_{kl}$  between the harmonic oscillator states corresponding to  $E^{(0)}$  and  $\mathbf{1}$  is the identity matrix with the dimension of the degenerate space.  $\mathcal{H}^{E^{(0)}}$  appears as a free Hamiltonian on the constraint surface coupled with the geometry induced gauge fields (28) and the potentials (18) and (29). Equation (26) have therefore to be interpreted as the Schrödinger equation describing the effective dynamics induced on the constraint surface. Note that for a surface  $\Sigma$  embedded in the three-dimensional euclidean space  $R^3$  the Hamiltonian (27) reduces to (2). We do not comment anymore on this fact referring to [4, 5] for details.

Denoting by  $\mathcal{K}$  the quantum numbers labelling the eigenfunctions of  $\mathcal{H}^{E^{(0)}}$  and supposed the degeneracy to be completely removed, the eigenvalues of  $\epsilon\mathcal{H}$  are evaluated by means of the standard formula

$$\epsilon\mathcal{E}_{\mathcal{N},\mathcal{K}} = E^{(0)} + \langle \mathcal{N}, \mathcal{K} | \mathcal{P}_\epsilon | \mathcal{N}, \mathcal{K} \rangle + \sum_{(\mathcal{N}', \mathcal{K}') \neq (\mathcal{N}, \mathcal{K})} \frac{|\langle \mathcal{N}, \mathcal{K} | \mathcal{P}_\epsilon | \mathcal{N}', \mathcal{K}' \rangle|^2}{E^{(0)} - E^{(0)'}} + \dots \quad (30)$$

This allows to calculate the spectrum of the system with an arbitrary accuracy as a power series in the parameter  $\epsilon$ .

## 5 Particle Constrained on a Circle

As a very simple but nontrivial example we consider a particle constrained to move on a circle embedded in  $R^3$  by an harmonic potential. This allows to illustrate some peculiarities of constrained quantomechanical systems which are systematically ignored in formal treatments. Let therefore be  $c : [0, 2\pi R] \rightarrow R^3$ ,  $c(x) = (R \cos(x/R), R \sin(x/R), 0)$  the embedding map of the circle in the three-dimensional euclidean space  $R^3$ . The curve is parametrized by the arclength  $x$ , so that its tangent, normal and binormal may be immediately evaluated as  $\mathbf{t}(x) = (-\sin(x/R), \cos(x/R), 0)$ ,  $\mathbf{n}(x) = (\cos(x/R), \sin(x/R), 0)$  and  $\mathbf{b}(x) = (0, 0, 1)$ . Every smooth assignment of an orthonormal basis of the normal space to  $c$  in  $x$  may be obtained by rotating normal and binormal by a point dependent angle  $w(x)$

$$\begin{aligned} \mathbf{n}^2 &= \cos w \mathbf{n} + \sin w \mathbf{b}, \\ \mathbf{n}^3 &= -\sin w \mathbf{n} + \cos w \mathbf{b}, \end{aligned} \quad (31)$$

where  $w(0) = w(2\pi R) + 2\pi z$ ,  $z$  being an integer. The induced metric, the second fundamental form and the normal fundamental form of the embedding read

$$\begin{aligned} g_{11} &= 1, \\ \alpha_{11}^2 &= \frac{1}{R_1} \cos w, \\ \alpha_{11}^3 &= -\frac{1}{R} \sin w, \\ A_1^{23} &= -\dot{w}. \end{aligned} \tag{32}$$

$\eta$  is so written as  $\eta = \frac{y^2}{R} \cos w - \frac{y^3}{R} \sin w$ , whereas the covariant derivative (19) on  $c$  reads  $\hat{\nabla}_x = \partial_x - i\dot{w}L_{23}$ . The direct calculation shows that  $\hat{\nabla}_x \eta = 0$ , so that the whole perturbative expansion (15) may be easily evaluated as

$$\begin{aligned} H^{(0)} &= \frac{1}{2} \left( -\partial_2^2 + \omega^2 y^{22} \right) + \frac{1}{2} \left( -\partial_3^2 + \omega^3 y^{32} \right), \\ H^{(1)} &= -\frac{1}{2} (\partial_x - i\dot{w}L_{23})^2 - \frac{1}{8R^2}, \\ &\dots, \\ H^{(N/2)} &= (N-1) \left( \frac{y^2}{R} \cos w - \frac{y^3}{R} \sin w \right)^{N-2} H^{(1)}, \\ &\dots \end{aligned} \tag{33}$$

The spectrum of the system may now be calculated by means of perturbation theory. As in the general case the infinite degeneracy of the zero order states is removed by solving the Schrödinger equation (26) for the effective dynamics on the constraint surface. In correspondence to the zero order state labelled by the harmonic oscillator quantum numbers  $(n_2, n_3)$  the effective Hamiltonian on the circle writes

$$\mathcal{H}^{(n_2, n_3)} = -\frac{1}{2} (\partial_x - i\dot{w}\langle L_{23} \rangle)^2 + \frac{1}{2} \left( \langle L_{23}^2 \rangle - \langle L_{23} \rangle^2 \right) \dot{w}^2 - \frac{1}{8R^2}, \tag{34}$$

where angled brackets denote again expectation values between harmonic oscillator states corresponding to the energy  $E^{(0)} = \omega^2(n_2 + 1/2) + \omega^3(n_3 + 1/2)$ .

Let us now discuss the physical meaning of the function  $w(x)$ . If the confining potential is symmetric, that is  $\omega^2 = \omega^3$ , it is possible to choose the harmonic oscillator basis in such a way that  $L_{23}$  is diagonal. The effective

potential  $(\langle L_{23}^2 \rangle - \langle L_{23} \rangle^2) \dot{w}^2 / 2$  vanishes then identically and  $\langle L_{23} \rangle \dot{w}$  appears then as a pure gauge field in the theory and may be removed by a different choice of normal coordinates  $y^2, y^3$ . The effective dynamics on the circle and the whole perturbative expansion result then considerably simplified. On the contrary, if the confining potential is not symmetric,  $\omega^2 \neq \omega^3$ ,  $\langle L_{23} \rangle = 0$ ,  $\langle L_{23}^2 \rangle \neq 0$  and a different choice of normal coordinates would cause the confining potential to be  $x$ -dependent. The effects produced by  $w(x)$  may therefore not be eliminated. Pictorially we may assimilate our model to a particle moving in a ring with a small ellipsoidal section. The function  $w(x)$  describes then how the section wraps up when moving along the ring. If the ring's section reduces to a circle ( $\omega^2 = \omega^3$ ) then does not matter how the wrapping is done and we are always reconduced to the case  $w = 0$ . On the contrary the wrapping produces observable effects when the ring's section is not circular ( $\omega^2 \neq \omega^3$ ).

The case  $\omega^2 = \omega^3$  being straightforward we concentrate on  $\omega^2 \neq \omega^3$ . The effective Hamiltonian describing the dynamics on the circle reduces then to

$$\mathcal{H}^{(n_2, n_3)} = -\frac{1}{2} \partial_x^2 + \frac{1}{2} \left[ \left( \frac{\omega^2}{\omega^3} + \frac{\omega^3}{\omega^2} \right) \left( n_2 + \frac{1}{2} \right) \left( n_3 + \frac{1}{2} \right) - \frac{1}{2} \right] \dot{w}^2 - \frac{1}{8R^2}. \quad (35)$$

Different choices of the *wrapping function*  $w(x)$  produce a completely different effective dynamics. An arbitrary positive, everywhere finite smooth potential may be reproduced by a suitable choice of  $w$ .

The simpler case we may consider is that in which the potential wraps us uniformly, say  $z$  times,  $w(x) = zx/R$ . The effective Schrödinger equation on the circle is then immediately solved by  $\phi_{(n_2, n_3), k}(x) = e^{i \frac{k}{R} x} / \sqrt{2\pi R}$ ,  $k$  any integer, and

$$E^{(1)} = \frac{1}{2R^2} \left\{ k^2 + z^2 \left[ \left( \frac{\omega^2}{\omega^3} + \frac{\omega^3}{\omega^2} \right) \left( n_2 + \frac{1}{2} \right) \left( n_3 + \frac{1}{2} \right) - \frac{1}{2} \right] - \frac{1}{4} \right\}. \quad (36)$$

Finer corrections to the spectrum may be evaluated by going over in perturbation theory. This matter not being particularly interesting for this model is postponed to the next example which is physically more significative. The remarkable fact we learn from this example is that the realization of the constraint, that is the particular form of the confining potential  $V_C$  characterizes the spectrum and the effective dynamics of the constrained quantum system. Such informations are completely lost within a formal treatment of the constraint.

## 6 Particle Constrained on a Sphere (The Rigid Diatom)

As a second example of a constrained quantomechanical system we consider the motion of a particle on a sphere embedded in  $R^3$ . To get some physical intuition on what we are dealing with let us consider a diatom. Aside from effects connected to the geometric phase [10], the effective Hamiltonian describing the rovibrational degrees of freedom of the molecule is written in the adiabatic approximation as

$$\mathcal{H}_{nuc} = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V_{BO}(|\mathbf{r}|), \quad (37)$$

where  $\mathbf{r} = (x, y, z)$  is the relative position of the nuclei,  $\mu$  the reduced mass of the system and  $V_{BO}$  is the Born-Oppenheimer potential. It is usual to assume that

- $V_{BO}$  presents a deep minimum in correspondence of the molecular equilibrium length  $r_0$ ,
- $V_{BO}$  depends only on the relative distance of the nuclei  $r = |\mathbf{r}|$  and not on the orientation of the molecule in space.

That is,  $V_{BO}$  behaves as a potential confining the motion from the rovibrational configuration space  $R^3$  to the sphere of radius  $r_0$ . Hamiltonian (37) describes therefore a constrained quantomechanical system in the sense we specified before, crf. (8).

In order to adapt coordinates we introduce the usual angles  $\theta$  and  $\phi$  parametrizing the sphere and the normal coordinate  $y = \frac{1}{r_0} \sqrt{\frac{I\omega}{\hbar}} (r - r_0)$ .  $I = \mu r_0^2$  is the momentum of inertia of the diatom and  $\omega$  the frequency introduced by the Born-Oppenheimer potential,  $\omega = \sqrt{\frac{2}{\mu} \frac{\partial^2 V_{BO}}{\partial r^2} |_{r=r_0}}$ . The adimensional scale factor  $\epsilon = \hbar/I\omega$  appears naturally in the definition of  $y$  once the zero order energy  $\hbar\omega$  is factorized from the Hamiltonian. From most diatoms  $\epsilon$  is a very small parameter,  $\epsilon \simeq 10^{-2} - 10^{-4}$ , and, as our notation anticipates, gives a measure of the rigidity of the molecule. The metric of  $R^3$  in the adapted coordinates frame reads

$$G_{IJ} = \frac{1}{\hbar\omega\epsilon} \begin{pmatrix} (1 + \epsilon^{1/2}y)^2 & 0 & 0 \\ 0 & (1 + \epsilon^{1/2}y)^2 \sin^2 \theta & 0 \\ 0 & 0 & \epsilon \end{pmatrix}, \quad (38)$$

while the Born-Oppenheimer potential writes as

$$V_{BO} = \hbar\omega \left( \frac{1}{2}y^2 + \hat{a}y^3 + \hat{b}y^4 + \dots \right), \quad (39)$$

where  $\hat{a} = a\hbar^{1/2}/\mu^{3/2}\omega^{5/2}$  and  $\hat{b} = b\hbar/\mu^2\omega^3$ ,  $a$  and  $b$  being the usual spectroscopical parameters. The rigidity parameter  $\hbar/I\omega$  plays therefore the rule of the parameter  $\epsilon$  we introduced in section 3 for a generic constraint<sup>1</sup>. A comparison of (38) with equations (5) and (6) allows to write down immediately the induced metric and the second fundamental form on the sphere

$$g_{\mu\nu} = \frac{1}{\hbar\omega\epsilon} \begin{pmatrix} 1 & 0 \\ 0 & \sin^2\theta \end{pmatrix}, \quad (40)$$

and

$$\alpha_{\mu\nu} = -\frac{\epsilon^{1/2}}{\hbar\omega} \begin{pmatrix} 1 & 0 \\ 0 & \sin^2\theta \end{pmatrix}. \quad (41)$$

The codimension of the constraint surface being one, the normal fundamental form vanishes identically. The embedding of the sphere in  $R^3$  is standard and the perturbative expansion  $\mathcal{H}/\hbar\omega = H^{(0)} + \epsilon H^{(1)} + \dots + \hat{a}y^3 + \hat{b}y^4 + \dots$  is easily evaluated as

$$\begin{aligned} H^{(0)} &= \frac{1}{2}(-\partial_y^2 + y^2), \\ H^{(1)} &= -\frac{1}{2} \left( \frac{1}{\sin\theta} \partial_\theta \sin\theta \partial_\theta + \frac{1}{\sin^2\theta} \partial_\phi^2 \right), \\ &\dots, \\ H^{(N/2)} &= (-1)^N (N-1) y^{N-2} H^{(1)}, \\ &\dots \end{aligned} \quad (42)$$

The zero order Hamiltonian  $H^{(0)}$  takes into account the vibrational motion of the diatom.  $H^{(1)}$  is the angular momentum operator describing the effective rotational dynamics as that of a spherical top. The rest of the perturbative expansion reproduces the Dunham expansion [11] of the nonrigid rotator taking into account rotovibrational interactions. The rotovibrational spectrum of the diatom finds therefore a very natural interpretation in terms of constrained quantum mechanics. Given up the classical idea of constraint

---

<sup>1</sup>Note that the normal coordinate  $y$  appears as already rescaled.

( $\epsilon \rightarrow 0$ ) the rovibrational structure appears naturally as a consequence of the physical structure of the constraint. The algorithm we present in this paper gives an automatic way to compute rovibrational interactions and may result usefull in the analysis of rigid polyatomic molecules [5]. For the moment we conclude by evaluating the spectrum of the particle constrained to the sphere. Introduced creation/destruction operators relative to the normal coordinate the computation results algebraic in nature and may be performed to an arbitrary order in perturbation theory by means of computer algebraic manipulation. We report here the expansion of the energy  $\mathcal{E}_{n,l}$  to the third order in perturbation theory

$$\begin{aligned} \frac{\mathcal{E}_{n,l}}{\hbar\omega} &= \left(n + \frac{1}{2}\right) + \epsilon \frac{1}{2} [l(l+1)] + \epsilon^2 \frac{3}{2} [l(l+1)] \left(n + \frac{1}{2}\right) + \\ &+ \epsilon^3 \left\{ \frac{15}{8} [l(l+1)] + \frac{15}{2} [l(l+1)] \left(n + \frac{1}{2}\right)^2 - \frac{1}{2} [l(l+1)]^2 \right\} + \\ &+ \left(\frac{3}{2}\hat{b} - 3\epsilon^{3/2}\hat{a} - \frac{15}{4}\hat{a}^2\right) \left(n + \frac{1}{2}\right)^2. \end{aligned} \quad (43)$$

Replacing the values of  $\epsilon$ ,  $\hat{a}$  and  $\hat{b}$  Eq.(43) reproduces the standard expression of rovibrational energies of diatoms [12].

## 7 Concluding Remarks

The reduction of the motion of a quantomechanical system from its configuration space to a submanifold is by no means unique, in the sense that it is impossible to perform this operation by completely disregarding the motion in the directions normal to the constraint surface. Quantum mechanics is a field theory, after all, and the wave function of the system keeps on exploring the whole configuration space even if squeezed on the constraint surface. When the system is in an eigenstate of the confining potential we can obtain an effective Hamiltonian describing the dynamics on the constraint surface. As is clearly illustrated by examples of sections 5 and 6 this effective dynamics, described by  $\mathcal{H}^{E^{(0)}}$ , depends both on the specific normal eigenstate and on the explicit form of the confining potential. In any case the eigenvalues of the effective Hamiltonian give only the first order corrections to the spectrum of the system at finite  $\epsilon$ . An accurate description requires also the analysis of the interaction between the motion normal and along the constraint surface.



The perturbative expansion (15) we present in this paper takes into account this effect.

Performing the limit  $\epsilon \rightarrow 0$  after subtracting the divergent zero order energies of the system produces a well defined description of the motion on the constraint surface. Nevertheless we consider this operation as artificial, the physical nature of the constraint being in the small but finite value of  $\epsilon$  (cfr. the discussion of the diatom). The whole perturbative expansion (15) is therefore necessary to characterize the dynamics of the constrained system.

Aside from its conceptual importance, the perturbative expansion (15) may reveal of practical importance in the analysis of electrons confined on arbitrary surfaces and wires as well as in the analysis of polyatomic molecular spectra. The effective rotational dynamics of some simple polyatomic molecules has already been considered in Ref.[5] demonstrating the physical relevance of the induced gauge structure and quantum potentials (28), (18) and (29). Our hope is that expansion (15) may serve as an unifying tool in understanding the fine structure spectra of rigid polyatomic molecules.

## Aknoledgments

I wish to warmly thank C. Destri and E. Onofri for useful discussions.

## References

- [1] P. A. M. Dirac, *Lectures notes on Quantum Mechanics*, (Yeshiva Press, New York, 1964)
- [2] B. De Witt, *Phys. Rev.* **85**, 635 (1952)
- [3] For a review see *The Quantum Hall Effect*, ed. R. E. Prange and S. M. Girvin (Springer-Verlag, 1989)
- [4] P. Maraner and C. Destri, *Mod. Phys. Lett.* **A8**, 9 861 (1993)
- [5] P. Maraner, *Parma University Preprint* UPRF-94-400
- [6] H. Jensen and H. Koppe, *Ann. of Phys.* **63**, 586 (1971)

- [7] R. A. Marcus, *J. Chem. Phys.* **45**, 4493 (1966); M. Kugler and S. Shtrikman, *Phys. Rev.* **D37**, 934 (1988); R. C. T. da Costa, *Phys. Rev.* **A23**, 1982 (1981); P. Exner, P. Seba and P. Stovicek, *Phys. Lett.* **A150**, 179 (1990); Y. Nagoshi and S. Takagi, *Jou. Phys.* **A24**, 4093 (1991); S. Takagi and T. Tanzawa, *Prog. Theo. Phys.* **87**, 561 (1992)
- [8] K. Fujii and N. Ogawa, *Prog. Theo. Phys.* **89**, 575 (1993)
- [9] See, for example, M. Spivak, *Differential Geometry* Vol. IV (Publich or Perich Inc., 1975)
- [10] J. Moody, A. Shpere and F. Wilczek, *Phys. Rev. Lett.* **56**, 9 199 (1986)
- [11] J. L. Dunham, *Phys. Rev.* **41**, 721 (1932)
- [12] G. Herzberg, *Molecular Spectra and Molecular Structure, I. Spectra of Diatomic Molecules* (Van Nostrand Reinhold Company, 1945)